Singular Value Decomposition

Note Title

LECTURE 13

- SVD is a matrix factorization that is useful for many applications, e.g., search engines, LS problems, tomographic image reconstruction, ...

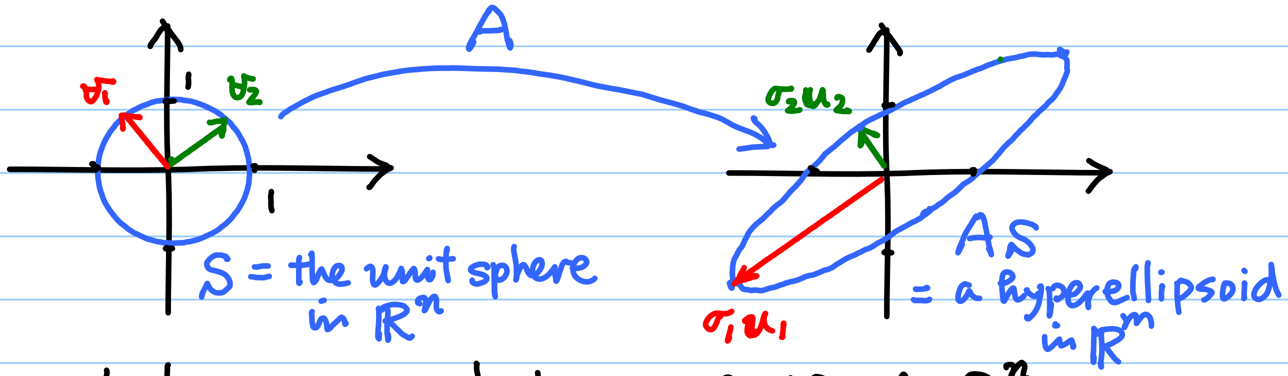
- SVD can be a concepual tool in linear algebra
  ⇒ via SVD, we can check:
  - a given matrix is near singular
  - rank of the matrix
  - etc.

- ∃ a numerically stable algorithm to compute the SVD of a given matrix (it's expensive though...)
  In fact, one of the hottest topics in numerical linear algebra is how to compute a good approximation to the SVD of a huge matrix fast!

☆ A Geometric Observation

Let $A \in \mathbb{R}^{m \times n}$, and consider how A maps an input vector in $\mathbb{R}^n$ to an output vector in $\mathbb{R}^m$.

"The image of the unit sphere under any $m \times n$ matrix is a hyperellipsoid"



ONB = orthonormal basis

Let $\{v_1, \cdots, v_n\}$ be an ONB of $\mathbb{R}^n$
Let $\{u_1, \cdots, u_m\}$ be an ONB of $\mathbb{R}^m$
Let $\{\sigma_1, \cdots, \sigma_m\}$ be a set of m scalars with $\sigma_i \geq 0$, $i = 1, \cdots m$.
Then, $\sigma_i u_i$ is the ith principal semiaxis with length σ_i in $\mathbb{R}^m$.

Now, if rank(A) = r, then exactly r of $\{\sigma_1, \cdots, \sigma_m\}$ are nonzero, and exactly m−r of σ_i's are zero.

So, if $\underline{m \geq n}$, then $\underline{\text{rank}(A) \leq n}$. ← full rank if = n
i.e., at most n of σ_i's are nonzero.

For simplicity, let's assume $m \geq n$ and rank(A) = n for the time being.

Def. The singular values of A
$\overset{\text{def}}{\Longleftrightarrow}$ The lengths of the n principal semiaxes of the hyperellipsoid AS

Our convention: $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \underset{\neq}{\geq} 0$

Def. The n left singular vectors of A $\overset{\text{def}}{\Longleftrightarrow}$ $\{u_1, \cdots, u_n\}$: the unit vectors

in $\mathbb{R}^m$ along the principal semiaxes of AS.
So, $\sigma_i u_i$ is the ith largest principal semiaxis of AS.

Def. The n right singular vectors of A $\overset{\text{def}}{\Longleftrightarrow}$ $\{v_1, \cdots, v_n\} \in S$: the preimages

of the principal semiaxes of AS, i.e.,

$$\underline{Av_i = \sigma_i u_i} \qquad i = 1, \cdots, n.$$

☆ Reduced SVD

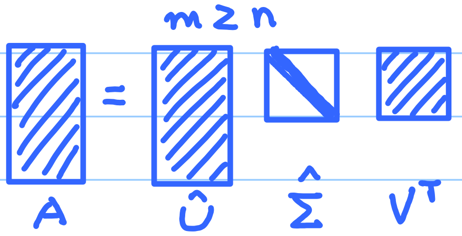
$$\underset{n}{{}^{m}\begin{bmatrix} A \end{bmatrix}} \underbrace{\begin{bmatrix} v_1 & \cdots & v_n \end{bmatrix}^{n}}_{\substack{n \\ \parallel \\ V}} = {}^{m}\underbrace{\begin{bmatrix} u_1 & \cdots & u_n \end{bmatrix}}_{\substack{n \\ \parallel \\ \hat{U}}} \underbrace{\begin{bmatrix} \sigma_1 & & 0 \\ & \ddots & \\ 0 & & \sigma_n \end{bmatrix}^{n}}_{\substack{n \\ \parallel \\ \hat{\Sigma}}}$$

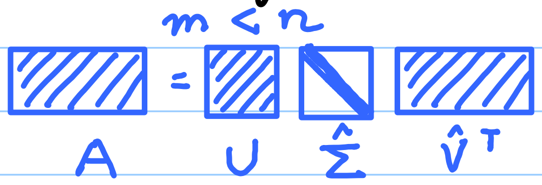
$$\Rightarrow \quad \underset{\substack{\uparrow \\ m\times n}}{A}\ \underset{\substack{\uparrow \\ n\times n}}{V} = \underset{\substack{\uparrow \\ m\times n}}{\hat{U}}\ \underset{\substack{\uparrow \\ n\times n}}{\hat{\Sigma}}$$

Since V is an orthogonal matrix,

$$\boxed{A = \hat{U}\hat{\Sigma}V^T}$$

The reduced SVD of A.





☆ Full SVD

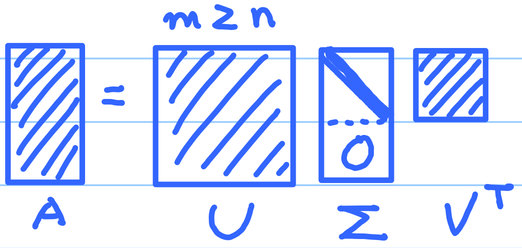
Note $\hat{U} \in \mathbb{R}^{m\times n}$ in the reduced SVD with $m \geq n$.

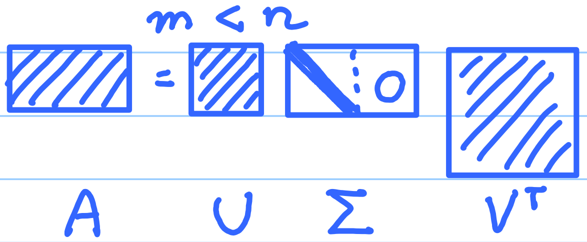
⇒ The column vectors of $\hat{U}$ do not form an ONB of $\mathbb{R}^m$ unless $m = n$.

⇒ Remedy : adjoin $m-n$ ON vectors to $\hat{U}$ to form an orthogonal matrix U. Then $\hat{\Sigma}$ must be changed to $\Sigma \in \mathbb{R}^{m\times n}$

$$\boxed{A = U \Sigma V^T}$$

The full SVD of A





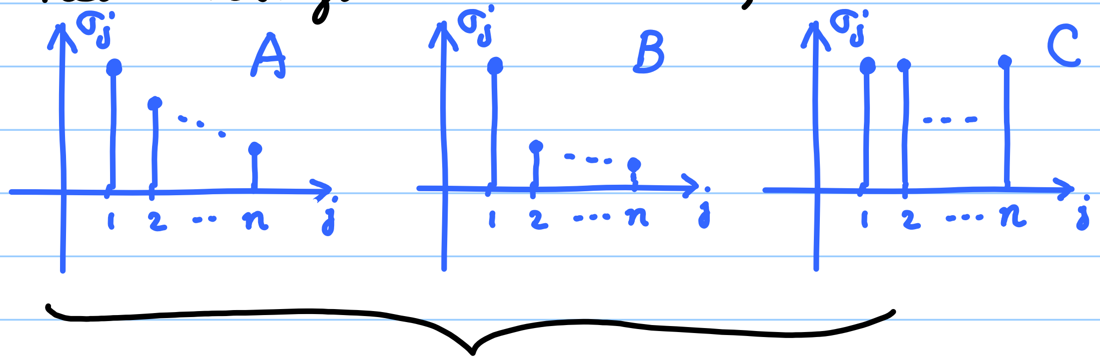
For non-full rank matrices, i.e., $\mathrm{rank}(A) = r < \min(m, n)$,
$\exists$ only r positive singular values.

So,

$$\Sigma = \underset{m \geq n}{\left[\begin{array}{c} \sigma_1 \ddots \sigma_r \; 0 \ddots 0 \\ \hdashline O \end{array}\right]} \text{ or } \underset{m \leq n}{\left[\begin{array}{c:c} \sigma_1 \ddots \sigma_r \; 0 \ddots 0 & O \end{array}\right]}$$

Let's consider $m = n$ and full rank case.
Theoretically, it's invertible, nonsingular.

However, we can gain more info by checking the distribution of the singular values of A ⇒ We can see whether A is near singular or not, etc.



Out of these three scenarios, which matrix do you think behaves best numerically?
⇒ C.

★ Pseudoinverse via SVD

$$\boxed{A^{+} = V \Sigma^{+} U^{T}}$$

where

$$\Sigma^{+} := \underset{m \ge n}{\left[\begin{array}{cccccc} \frac{1}{\sigma_1} & & & & & \\ & \ddots & & & & \\ & & \frac{1}{\sigma_r} & & & \\ & & & 0 & & \\ & & & & \ddots & \\ & & & & & 0 \\ \hdashline & & & O & & \end{array}\right]} \text{ or } \underset{m \le n}{\left[\begin{array}{cccccc:c} \frac{1}{\sigma_1} & & & & & & \\ & \ddots & & & & & \\ & & \frac{1}{\sigma_r} & & & & O \\ & & & 0 & & & \\ & & & & \ddots & & \\ & & & & & 0 & \end{array}\right]}$$

Check:

$$\begin{aligned} AA^{+} &= U\Sigma V^{T} V \Sigma^{+} U^{T} \\ &= U \Sigma \Sigma^{+} U^{T} \\ &= U \begin{bmatrix} 1 & & & & & \\ & \ddots & & & & \\ & & 1 & & & \\ & & & 0 & & \\ & & & & \ddots & \\ & & & & & 0 \\ \hline & & O & & & \end{bmatrix} U^{T} \\ &= \begin{bmatrix} u_1 & \cdots & u_r & 0 & \cdots & 0 \end{bmatrix} \begin{bmatrix} u_1^{T} \\ \vdots \\ u_m^{T} \end{bmatrix} \\ &= \underset{\sim}{\hat{U}} \, \underset{\sim}{\hat{U}}^{T} \end{aligned}$$

$\longrightarrow$ reduced version.

Similarly, $A^{+}A = \underset{\sim}{\hat{V}} \, \underset{\sim}{\hat{V}}^{T}$

The Moore-Penrose Conditions

For a given matrix $A \in \mathbb{R}^{m \times n}$, if $X \in \mathbb{R}^{n \times m}$ satisfies the following:

$$\begin{cases} (1) & AXA = A \\ (2) & XAX = X \\ (3) & (AX)^{T} = AX \\ (4) & (XA)^{T} = XA \end{cases}$$

then X is called the pseudoinverse (or the Moore-Penrose inverse) of A and written as A^{+}

$\exists$ many applications using A^{+}!

Note: If $\| AX - I_m \|_F \to \min$ then $X = A^{+}$.